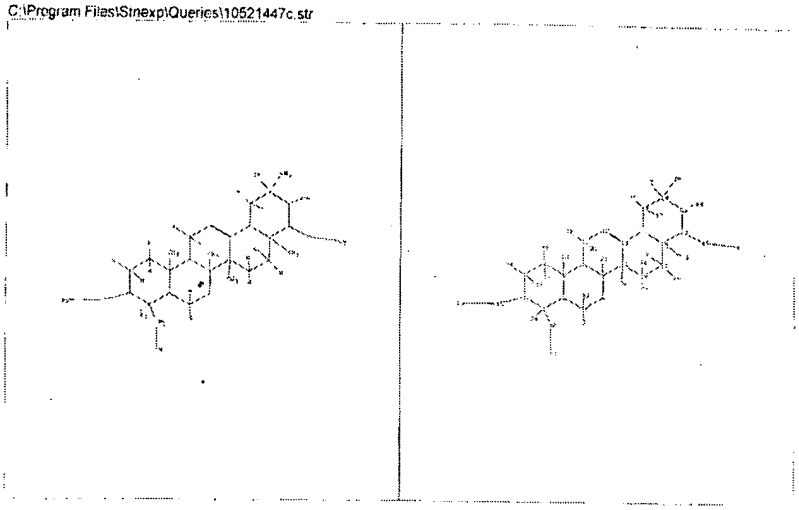
C:\Program Files\Stnexp\Queries\10521447c.str



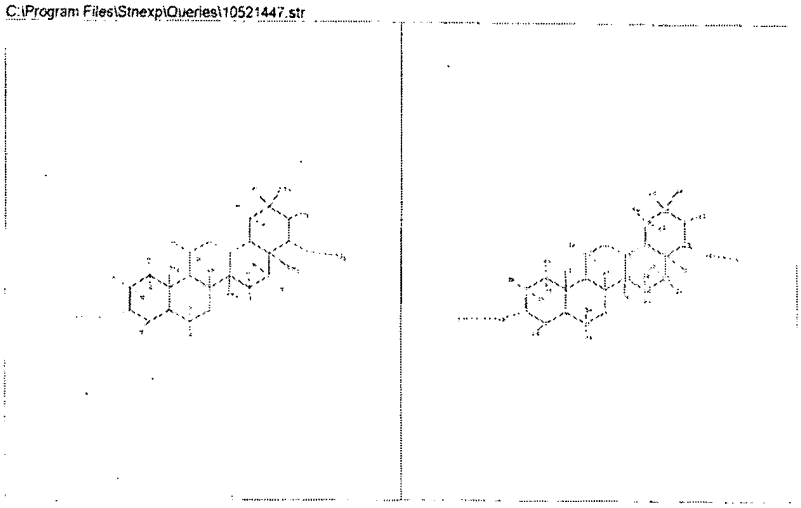
chain nodes :
23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 43 44 45 46 47 49 50 52 53
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
1-24 1-52 2-45 3-38 3-39 4-40 4-41 5-23 8-25 10-30 10-31 11-32 11-33 14-26 16-27 17-36 17-37 18-34 18-35 19-46 19-47 20-28 20-29 21-43 22-44 44-50 45-49 52-53
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14 13-15 14-18 15-16 15-19 16-17 18-22 17-18 19-20 20-21 21-22
exact/norm bonds :
1-2 1-6 2-3 2-45 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14 13-15 14-18 15-16 15-19 16-17 16-22 17-18 19-20 20-21 21-22 21-43 22-44 44-50 45-49
exact bonds :
1-24 1-52 3-38 3-39 4-40 4-41 5-23 8-25 10-30 10-31 11-32 11-33 14-26 16-27 17-36 17-37 18-34 18-35 19-46 19-47 20-28 20-29 52-53

G1:H,OH

G2:H,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS24:CLASS25:CLASS26:CLASS27:CLASS28:CLASS29:CLASS30:CLASS31:CLASS32:CLASS33:CLASS34:CLASS35:CLASS36:CLASS37:CLASS38:CLASS39:CLASS40:CLASS41:CLASS43:CLASS44:CLASS45:CLASS46:CLASS47:CLASS49:CLASS50:CLASS52:CLASS53:CLASS

C:\Program Files\Stnexp\Queries\10521447.str



chain nodes :
23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 43 44 45 46 47 49 50
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
1-24 2-45 3-38 3-39 4-40 4-41 5-23 8-25 10-30 10-31 11-32 11-33 14-26 16-27 17-36 17-37 18-34 18-35 19-46 19-47 20-28 20-29 21-43 22-44 44-50 45-49
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14 13-15 14-18 15-16 15-19 16-17 16-22 17-18 19-20 20-21 21-22
exact/norm bonds :
1-2 1-6 2-3 2-45 3-4 3-38 3-39 4-5 4-40 4-41 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 10-30 10-31 11-12 11-32 11-33 12-13 13-14 13-15 14-18 15-16 15-19 16-17 16-22 17-18 17-36 17-37 18-34 18-35 19-20 19-46 19-47 20-21 21-22 21-43 22-44 44-50 45-49
exact bonds :
1-24 5-23 8-25 14-26 16-27 20-28 20-29

G1:H,OH

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS24:CLASS25:CLASS26:CLASS 27:CLASS28:CLASS29:CLASS30:CLASS31:CLASS32:CLASS33:CLASS34:CLASS35:CLASS36:CLASS37:CLASS38:CLASS 39:CLASS40:CLASS41:CLASS43:CLASS44:CLASS45:CLASS46:CLASS47:CLASS49:CLASS50:CLASS

10/523,417

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     FILE 'REGISTRY' ENTERED AT 09:02:47 ON 02 APR 2007
L1              STRUCTURE UPLOADED
L2            14 S L1 SSS SAM
L3              STRUCTURE UPLOADED
L4             ? S L3 SSS SAM
L5            ?? S L3 FULL
L6              STRUCTURE UPLOADED
L7             ? S L6 FULL

     FILE 'CAPLUS' ENTERED AT 09:08:10 ON 02 APR 2007
L8            ?? S L?
L9            15 S L5

     FILE 'REGISTRY' ENTERED AT 09:11:54 ON 02 APR 2007
L10             STRUCTURE UPLOADED
L11            ? S L10 SSS SAM
L12           ?? S L10 FULL
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Btcsh